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# Methyl 2-[(*tert*-butoxycarbonyl)amino]-3-(4-hydroxyphenyl)propanoate

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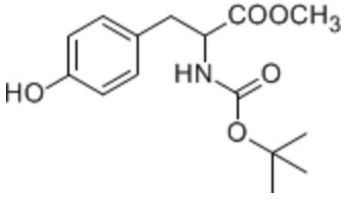
Key indicators: single-crystal X-ray study; $T$ = 100 K; mean $\sigma$(C–C) = 0.002 Å; $R$ factor = 0.039; $wR$ factor = 0.102; data-to-parameter ratio = 19.1.

In the title molecule, $C_{15}H_{21}NO_5$, the dihedral angle between the mean plane of the –N—C(=O)—O– group [maximum deviation = 0.002 (1) Å for the C atom] and the benzene ring is 82.2 (2)°. In the crystal, O—H···O and N—H···O hydrogen bonds connect the molecules, forming a two-dimensional network parallel to (001).

## Related literature

For the biological activity of related compounds, see: Sykes *et al.* (1999).




## Experimental

### Crystal data

$C_{15}H_{21}NO_5$
$M_r$ = 295.33
Orthorhombic, $P2_12_12_1$
$a$ = 8.7879 (8) Å
$b$ = 9.4844 (9) Å
$c$ = 18.9207 (18) Å
$V$ = 1577.0 (3) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 0.09 mm$^{-1}$
$T$ = 100 K
0.55 × 0.49 × 0.45 mm

### Data collection

Bruker APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min}$ = 0.962, $T_{max}$ = 0.989
9339 measured reflections
3636 independent reflections
3469 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.072

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.102
$S$ = 1.03
3636 reflections
190 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.32 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.20 e Å$^{-3}$

**Table 1**
Hydrogen-bond geometry (Å, °).

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| N1—H1$B$···O3$^{i}$ | 0.86 | 2.27 | 3.0583 (16) | 153 |
| O1—H1$C$···O5$^{ii}$ | 0.82 | 1.92 | 2.7356 (15) | 180 |

Symmetry codes: (i) $x+\frac{1}{2}, -y+\frac{3}{2}, -z$; (ii) $x, y+1, z$.

Data collection: *APEX2* (Bruker, 2007); cell refinement: *APEX2*; data reduction: *SAINT* (Bruker, 2007)'; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL* and *PLATON* (Spek, 2009); software used to prepare material for publication: *SHELXTL* and *publCIF* (Westrip, 2010).

The author thanks Henan University of Traditional Chinese Medicine for supporting this study.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LH5632).

## References

Bruker (2007). *APEX2* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Spek, A. L. (2009). *Acta Cryst.* D**65**, 148–155.
Sykes, B. M., Atwell, G. J., Hogg, A., Wilson, W. R., O'Connor, C. J. & Denny, W. A. (1999). *J. Med. Chem.* **42**, 346-355.
Westrip, S. P. (2010). *J. Appl. Cryst.* **43**, 920–925.

# supporting information

*Acta Cryst.* (2013). E**69**, o1372 [doi:10.1107/S160053681301979X]

## Methyl 2-[(*tert*-butoxycarbonyl)amino]-3-(4-hydroxyphenyl)propanoate

**Xiaokun Li**

### S1. Comment

Amide, ester and hydroxyl groups widely exist in many biologically active compounds or can be utilized in prodrugs (Sykes *et al.*, 1999). Herein we report the crystal structure of the title compound. The dihedral angle between the mean-plane of the amide group (N1/C9/O5/O4) [a maximum deviation of 0.002 (1)° for C9) and the benzene ring (C1–C6) is 82.2 (2)°. In the crystal, O—H···O and N—H···O hydrogen bonds connect molecules forming a two-dimensional network parallel to (001) (Fig. 2).

### S2. Experimental

The title compound (0.3 mmol, 88.5 mg) was dissolved in 10 ml of methanol solution. Colorless block-shaped crystals separated after 5 d.

### S3. Refinement

H atoms were included in calculated positions and treated as riding atoms: C—H = 0.93, 0.96 and 0.98 Å for CH(aromatic), $CH_3$ and CH(methine) H atoms, respectively, or N—H = 0.86 Å and O—H = 0.82 Å with $U_{iso}$(H)= $kU_{eq}$(parent C-atom, N), where k = 1.5 for $CH_3$ and hydroxyl H atoms and k = 1.2 for all other H atoms. The absolute congiuration could not be determined from the X-ray data. In the absence of anamolous dispersion effects Friedel pairs were merged.

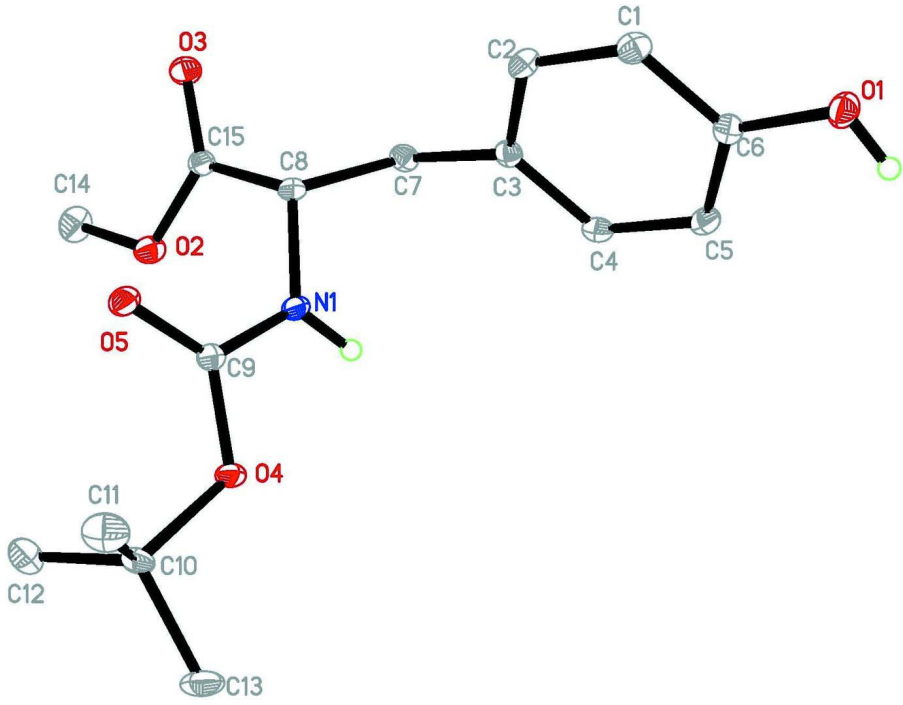



**Figure 1**

The molecular strcuture of the title compound with displacement ellipsoids drawn at the 30% probability level.

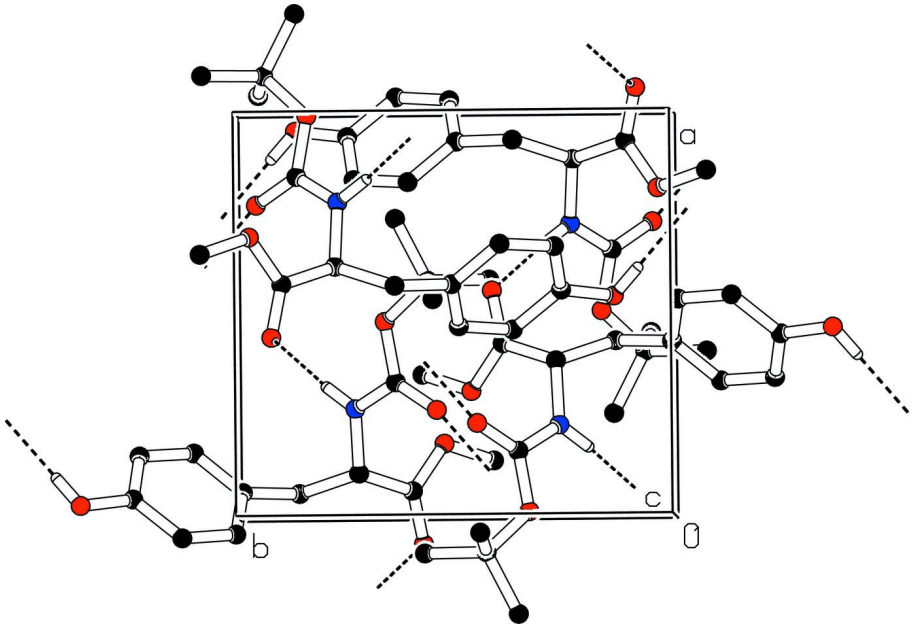



**Figure 2**

Part of the crystal structure with hydrogen bonds shown as dashed lines. H atoms bonded to C atoms are not shown.

**Methyl 2-[(*tert*-butoxycarbonyl)amino]-3-(4-hydroxyphenyl)propanoate**

*Crystal data*

$C_{15}H_{21}NO_5$
$M_r = 295.33$
Orthorhombic, $P2_12_12_1$
Hall symbol: P 2ac 2ab
$a = 8.7879$ (8) Å
$b = 9.4844$ (9) Å
$c = 18.9207$ (18) Å
$V = 1577.0$ (3) Å$^3$
$Z = 4$
$F(000) = 632$
$D_x = 1.244$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 9371 reflections
$\theta = 1.0$–$27.6°$
$\mu = 0.09$ mm$^{-1}$
$T = 100$ K
Block, colourless
0.55 × 0.49 × 0.45 mm

*Data collection*

Bruker APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\varphi$ and $\omega$ scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.962$, $T_{max} = 0.989$
9339 measured reflections
3636 independent reflections
3469 reflections with $I > 2\sigma(I)$
$R_{int} = 0.072$
$\theta_{max} = 27.6°$, $\theta_{min} = 2.2°$
$h = -11 \rightarrow 9$
$k = -12 \rightarrow 8$
$l = -24 \rightarrow 24$

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.039$
$wR(F^2) = 0.102$
$S = 1.03$
3636 reflections
190 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0581P)^2 + 0.1712P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.008$
$\Delta\rho_{max} = 0.32$ e Å$^{-3}$
$\Delta\rho_{min} = -0.20$ e Å$^{-3}$

*Special details*

**Geometry**. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

**Refinement**. Refinement of $F^2$ against ALL reflections. The weighted $R$-factor $wR$ and goodness of fit $S$ are based on $F^2$, conventional $R$-factors $R$ are based on $F$, with $F$ set to zero for negative $F^2$. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating $R$-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. $R$-factors based on $F^2$ are statistically about twice as large as those based on $F$, and $R$-factors based on ALL data will be even larger.

*Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å$^2$)*

| | $x$ | $y$ | $z$ | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| C1 | −0.04196 (17) | 1.13511 (15) | 0.18071 (7) | 0.0216 (3) |
| H1A | −0.1123 | 1.1434 | 0.2172 | 0.026* |
| C2 | −0.03335 (16) | 1.01206 (15) | 0.14197 (7) | 0.0205 (3) |
| H2A | −0.0978 | 0.9376 | 0.1531 | 0.025* |
| C3 | 0.07017 (15) | 0.99675 (14) | 0.08627 (7) | 0.0172 (3) |

| | | | | |
|---|---|---|---|---|
| C4 | 0.16908 (15) | 1.10800 (15) | 0.07254 (7) | 0.0192 (3) |
| H4A | 0.2409 | 1.0991 | 0.0367 | 0.023* |
| C5 | 0.16250 (16) | 1.23229 (15) | 0.11142 (7) | 0.0200 (3) |
| H5A | 0.2297 | 1.3055 | 0.1016 | 0.024* |
| C6 | 0.05528 (16) | 1.24689 (14) | 0.16488 (7) | 0.0184 (3) |
| C7 | 0.06700 (17) | 0.86702 (15) | 0.04022 (7) | 0.0188 (3) |
| H7A | 0.1336 | 0.8823 | 0.0001 | 0.023* |
| H7B | −0.0354 | 0.8547 | 0.0221 | 0.023* |
| C8 | 0.11575 (14) | 0.73007 (14) | 0.07772 (7) | 0.0166 (3) |
| H8A | 0.0573 | 0.7217 | 0.1216 | 0.020* |
| C9 | 0.33960 (15) | 0.64306 (14) | 0.13963 (7) | 0.0159 (3) |
| C10 | 0.59030 (15) | 0.56854 (15) | 0.18449 (7) | 0.0199 (3) |
| C11 | 0.5429 (2) | 0.5555 (2) | 0.26171 (8) | 0.0302 (3) |
| H11A | 0.5434 | 0.6471 | 0.2833 | 0.045* |
| H11B | 0.6131 | 0.4950 | 0.2861 | 0.045* |
| H11C | 0.4424 | 0.5161 | 0.2644 | 0.045* |
| C12 | 0.59178 (18) | 0.42703 (17) | 0.14678 (8) | 0.0280 (3) |
| H12A | 0.6225 | 0.4403 | 0.0985 | 0.042* |
| H12B | 0.4917 | 0.3866 | 0.1480 | 0.042* |
| H12C | 0.6621 | 0.3649 | 0.1699 | 0.042* |
| C13 | 0.74355 (17) | 0.64103 (19) | 0.17817 (9) | 0.0305 (3) |
| H13A | 0.7714 | 0.6480 | 0.1292 | 0.046* |
| H13B | 0.8190 | 0.5872 | 0.2030 | 0.046* |
| H13C | 0.7373 | 0.7338 | 0.1982 | 0.046* |
| C14 | 0.1469 (2) | 0.42237 (17) | −0.04498 (8) | 0.0292 (3) |
| H14A | 0.2370 | 0.3749 | −0.0609 | 0.044* |
| H14B | 0.0943 | 0.4618 | −0.0848 | 0.044* |
| H14C | 0.0816 | 0.3563 | −0.0213 | 0.044* |
| C15 | 0.07176 (16) | 0.60783 (14) | 0.02939 (7) | 0.0180 (3) |
| N1 | 0.27499 (13) | 0.73700 (12) | 0.09567 (6) | 0.0170 (2) |
| H1B | 0.3301 | 0.8029 | 0.0778 | 0.020* |
| O1 | 0.04029 (13) | 1.36708 (11) | 0.20398 (5) | 0.0247 (2) |
| H1C | 0.1090 | 1.4220 | 0.1939 | 0.037* |
| O2 | 0.18880 (11) | 0.53485 (11) | 0.00379 (5) | 0.0221 (2) |
| O3 | −0.05943 (13) | 0.58394 (11) | 0.01458 (6) | 0.0254 (2) |
| O4 | 0.48955 (11) | 0.66726 (10) | 0.14566 (5) | 0.0186 (2) |
| O5 | 0.27010 (12) | 0.54940 (10) | 0.16994 (5) | 0.0204 (2) |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| C1 | 0.0215 (7) | 0.0263 (7) | 0.0171 (6) | −0.0023 (6) | 0.0044 (5) | 0.0007 (5) |
| C2 | 0.0205 (6) | 0.0205 (6) | 0.0206 (6) | −0.0054 (5) | 0.0015 (5) | 0.0015 (5) |
| C3 | 0.0161 (6) | 0.0182 (6) | 0.0172 (6) | 0.0019 (5) | −0.0039 (5) | 0.0011 (5) |
| C4 | 0.0145 (6) | 0.0235 (7) | 0.0195 (6) | 0.0009 (5) | 0.0020 (5) | 0.0009 (5) |
| C5 | 0.0176 (6) | 0.0208 (6) | 0.0217 (6) | −0.0034 (5) | 0.0006 (5) | 0.0018 (5) |
| C6 | 0.0200 (6) | 0.0185 (6) | 0.0167 (5) | −0.0002 (5) | −0.0023 (5) | 0.0006 (5) |
| C7 | 0.0179 (6) | 0.0208 (6) | 0.0178 (6) | 0.0018 (5) | −0.0025 (5) | −0.0009 (5) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C8 | 0.0116 (6) | 0.0203 (6) | 0.0178 (6) | −0.0004 (5) | −0.0014 (5) | −0.0005 (5) |
| C9 | 0.0152 (6) | 0.0171 (6) | 0.0155 (5) | −0.0002 (5) | 0.0007 (5) | −0.0038 (5) |
| C10 | 0.0145 (6) | 0.0248 (7) | 0.0206 (6) | 0.0027 (5) | −0.0050 (5) | 0.0017 (5) |
| C11 | 0.0281 (8) | 0.0429 (9) | 0.0196 (6) | 0.0005 (7) | −0.0040 (6) | 0.0012 (6) |
| C12 | 0.0281 (8) | 0.0264 (7) | 0.0296 (7) | 0.0064 (6) | −0.0033 (6) | 0.0000 (6) |
| C13 | 0.0146 (7) | 0.0421 (9) | 0.0348 (8) | −0.0032 (6) | −0.0069 (6) | 0.0052 (7) |
| C14 | 0.0364 (9) | 0.0281 (7) | 0.0232 (7) | −0.0031 (7) | 0.0026 (6) | −0.0084 (6) |
| C15 | 0.0164 (6) | 0.0189 (6) | 0.0188 (6) | −0.0003 (5) | −0.0011 (5) | 0.0037 (5) |
| N1 | 0.0129 (5) | 0.0185 (5) | 0.0196 (5) | −0.0023 (4) | −0.0008 (4) | 0.0012 (4) |
| O1 | 0.0269 (5) | 0.0215 (5) | 0.0256 (5) | −0.0057 (4) | 0.0063 (4) | −0.0059 (4) |
| O2 | 0.0191 (5) | 0.0249 (5) | 0.0224 (5) | −0.0012 (4) | 0.0020 (4) | −0.0060 (4) |
| O3 | 0.0179 (5) | 0.0250 (5) | 0.0333 (5) | −0.0016 (4) | −0.0080 (4) | −0.0020 (4) |
| O4 | 0.0123 (4) | 0.0210 (5) | 0.0223 (4) | −0.0010 (3) | −0.0038 (4) | 0.0031 (4) |
| O5 | 0.0175 (5) | 0.0214 (5) | 0.0221 (4) | −0.0027 (4) | 0.0013 (4) | 0.0028 (4) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| C1—C2 | 1.380 (2) | C10—O4 | 1.4834 (16) |
| C1—C6 | 1.3942 (19) | C10—C13 | 1.517 (2) |
| C1—H1A | 0.9300 | C10—C12 | 1.520 (2) |
| C2—C3 | 1.3997 (19) | C10—C11 | 1.524 (2) |
| C2—H2A | 0.9300 | C11—H11A | 0.9600 |
| C3—C4 | 1.3915 (19) | C11—H11B | 0.9600 |
| C3—C7 | 1.5079 (18) | C11—H11C | 0.9600 |
| C4—C5 | 1.391 (2) | C12—H12A | 0.9600 |
| C4—H4A | 0.9300 | C12—H12B | 0.9600 |
| C5—C6 | 1.3893 (19) | C12—H12C | 0.9600 |
| C5—H5A | 0.9300 | C13—H13A | 0.9600 |
| C6—O1 | 1.3653 (16) | C13—H13B | 0.9600 |
| C7—C8 | 1.5408 (19) | C13—H13C | 0.9600 |
| C7—H7A | 0.9700 | C14—O2 | 1.4578 (17) |
| C7—H7B | 0.9700 | C14—H14A | 0.9600 |
| C8—N1 | 1.4415 (16) | C14—H14B | 0.9600 |
| C8—C15 | 1.5265 (18) | C14—H14C | 0.9600 |
| C8—H8A | 0.9800 | C15—O3 | 1.2079 (18) |
| C9—O5 | 1.2210 (17) | C15—O2 | 1.3309 (17) |
| C9—O4 | 1.3424 (16) | N1—H1B | 0.8600 |
| C9—N1 | 1.3447 (17) | O1—H1C | 0.8200 |
| | | | |
| C2—C1—C6 | 119.69 (13) | O4—C10—C11 | 111.29 (12) |
| C2—C1—H1A | 120.2 | C13—C10—C11 | 110.79 (12) |
| C6—C1—H1A | 120.2 | C12—C10—C11 | 112.37 (13) |
| C1—C2—C3 | 121.55 (13) | C10—C11—H11A | 109.5 |
| C1—C2—H2A | 119.2 | C10—C11—H11B | 109.5 |
| C3—C2—H2A | 119.2 | H11A—C11—H11B | 109.5 |
| C4—C3—C2 | 117.90 (12) | C10—C11—H11C | 109.5 |
| C4—C3—C7 | 121.49 (12) | H11A—C11—H11C | 109.5 |
| C2—C3—C7 | 120.51 (12) | H11B—C11—H11C | 109.5 |

| | | | |
|---|---|---|---|
| C5—C4—C3 | 121.20 (12) | C10—C12—H12A | 109.5 |
| C5—C4—H4A | 119.4 | C10—C12—H12B | 109.5 |
| C3—C4—H4A | 119.4 | H12A—C12—H12B | 109.5 |
| C6—C5—C4 | 119.85 (12) | C10—C12—H12C | 109.5 |
| C6—C5—H5A | 120.1 | H12A—C12—H12C | 109.5 |
| C4—C5—H5A | 120.1 | H12B—C12—H12C | 109.5 |
| O1—C6—C5 | 122.90 (12) | C10—C13—H13A | 109.5 |
| O1—C6—C1 | 117.34 (12) | C10—C13—H13B | 109.5 |
| C5—C6—C1 | 119.75 (12) | H13A—C13—H13B | 109.5 |
| C3—C7—C8 | 114.62 (10) | C10—C13—H13C | 109.5 |
| C3—C7—H7A | 108.6 | H13A—C13—H13C | 109.5 |
| C8—C7—H7A | 108.6 | H13B—C13—H13C | 109.5 |
| C3—C7—H7B | 108.6 | O2—C14—H14A | 109.5 |
| C8—C7—H7B | 108.6 | O2—C14—H14B | 109.5 |
| H7A—C7—H7B | 107.6 | H14A—C14—H14B | 109.5 |
| N1—C8—C15 | 114.93 (11) | O2—C14—H14C | 109.5 |
| N1—C8—C7 | 109.87 (11) | H14A—C14—H14C | 109.5 |
| C15—C8—C7 | 107.10 (10) | H14B—C14—H14C | 109.5 |
| N1—C8—H8A | 108.2 | O3—C15—O2 | 123.75 (13) |
| C15—C8—H8A | 108.2 | O3—C15—C8 | 121.54 (12) |
| C7—C8—H8A | 108.2 | O2—C15—C8 | 114.67 (11) |
| O5—C9—O4 | 125.14 (13) | C9—N1—C8 | 121.70 (11) |
| O5—C9—N1 | 124.15 (13) | C9—N1—H1B | 119.2 |
| O4—C9—N1 | 110.71 (12) | C8—N1—H1B | 119.2 |
| O4—C10—C13 | 101.82 (11) | C6—O1—H1C | 109.5 |
| O4—C10—C12 | 109.26 (11) | C15—O2—C14 | 114.55 (12) |
| C13—C10—C12 | 110.83 (13) | C9—O4—C10 | 121.33 (11) |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N1—H1*B*···O3$^{i}$ | 0.86 | 2.27 | 3.0583 (16) | 153 |
| O1—H1*C*···O5$^{ii}$ | 0.82 | 1.92 | 2.7356 (15) | 180 |

Symmetry codes: (i) $x+1/2, -y+3/2, -z$; (ii) $x, y+1, z$.